

1,3-Dioxolane  
646-06-0 | DTXSID4027284

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 5.55e-12 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 6.76e-01

**Confidence level:** 7.43e-01

## Nearest Neighbors from the Training Set

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1,4-Dioxane

**Measured:** 1.09e-11

**Predicted:** 7.30e-12

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2-Chloroethanol

**Measured:** 1.40e-12

**Predicted:** 2.40e-12

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Dimethoxymethane

**Measured:** 4.90e-12

**Predicted:** 6.85e-12

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1,3-Dioxane

**Measured:** 9.15e-12

**Predicted:** 1.03e-11

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2-Methyl-1,3-dioxolane

**Measured:** 9.40e-12

**Predicted:** 9.84e-12